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From observations to abundances:

equivalent widths and line profile fitting

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Abstract.
Modern spectral analysis relies on the comparison between observations and theoretical computations. In this contribution I focus on how this comparison is performed. I address the problem of estimating errors and argue that the preferred method is through Monte Carlo simulations. I analyse the effect of rebinning spectra to a constant wavelength step and show that it is possible to analyse spectra also without resorting to rebinning. The "no rebinning" approach allows to efficiently combine spectra of different binning without any loss of information.

Key words. Methods:data analysis - Techniques: spectroscopic - Stars: abundances

1. Observed spectra

Let us start by recalling briefly what is the data that one deals with, when analyzing a spectrum. In an astronomical spectrograph the photons are dispersed and then focused onto a detector, which in most cases, is a two-dimensional array of pixels. What is recorded is a signal, which for linear detectors is proportional to the number of incoming photons, in each pixel, this signal is output as a number. The goal of data-reduction is to transform this two dimensional array of numbers into a one dimensional array which gives the flux as a function of wavelength $S_{ij} \mapsto f(\lambda_k)$. The entrance slit of the spectrograph projects onto the focal plane in a way which is determined by the optics of the spectrograph. The simplest case is that a rectangular slit of $X'' \times Y''$ on the sky projects onto a rectangular slit on the focal plane of $x \times y$, where x and y are expressed in pixels (here and after we assume x along the dispersion direction and y perpendicular). If $x < 2$ the spectrum is undersampled and the resolution is fixed by the pixel size. In all other cases the resolution is fixed by the slit width. In general a rectangular slit does not project as a rectangle on the focal plane, but there is curvature, i.e. if pixel (i, j) corresponds to wavelength λ pixels $(i, j+1)$ and $(i, j-1)$ do not correspond to the same λ but to two other distinct wavelengths. The correspondence between pixel and wavelength(the "wavelength solution") is obtained from the spectrum of a lamp in which lines of known laboratory wave-

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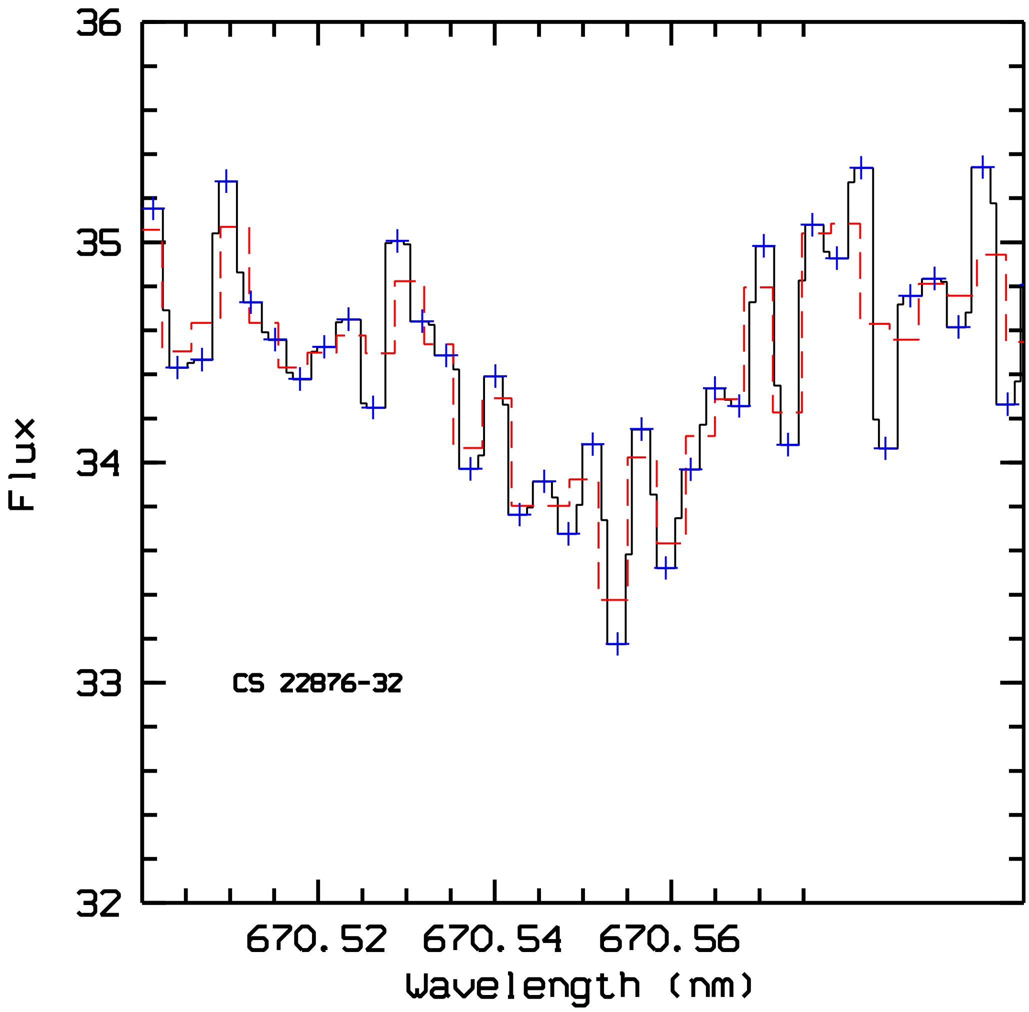

Fig. 1. A portion of a UVES spectrum of CS22876-32. The crosses are the non-rebinned pixel values, the solid line is the data rebinned with oversampling with a step of 0.007 Å, while the dotted line is rebinned with a pixel size, slightly larger than the largest physical pixel size, 0.033 Å. It is clear that oversampling preserves the resolution, while non-oversampling does not.

lengths can be identified. So we determine a correspondence $(i, j) \mapsto \lambda_{i,j}$. The common practice is to "extract the spectrum", i.e. add up the flux contained in all the pixels which correspond to the same wavelength. If there is non-negligible curvature along the slit no pair of pixels will correspond to the same wavelength, therefore in order to make this possible one has to "rebin" the spectra, in order to avoid loss of spectral resolution one usually does this by oversampling, i.e. introducing a virtual grid whose pixel size is typically 1/2 or 1/3 of the real pixel size. An example of a real UVES spectrum, shown in Fig.1 demonstrates that if one does not oversample the spectrum, when rebinning, there is some loss of resolution. This virtual grid has a constant step in wavelength and the transformation corrects the slit curvature so that now all pixels with the same wavelength may be added up directly

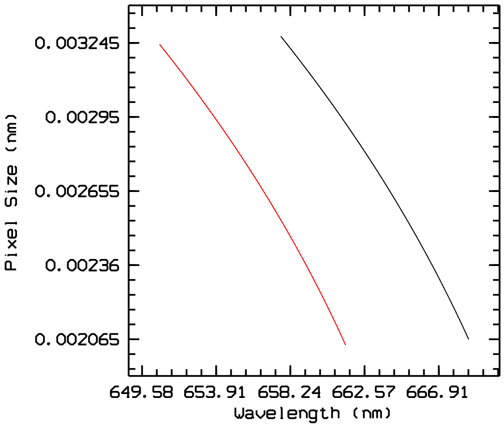

Fig. 2. The pixel size in nm along two orders in the 573nm setting.

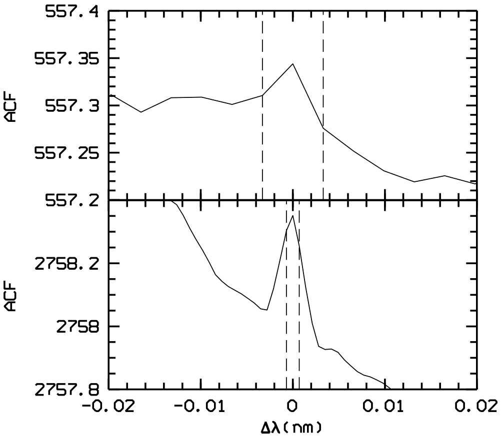

Fig. 3. The auto-correlation functions for the spectrum in figure 1, with oversampling (bottom panel) and no oversampling (top panel). In both panels vertical dotted lines delimit twice the pixel size. It is clear that with oversampling the pixels are correlated.

(with suitable weights, if necessary, in this case one talks about "optimal extraction"). Even in cases when the slit curvature is negligible, so that the projected slit is effectively rectangular, it is common practice to rebin the spectra at steps of constant wavelength. This allows for instance: 1) to co-add different spectra of the same object; 2) merge echelle orders with non-negligible overlap. In some echelle spectrographs like UVES, in which the anamorphism produces a variable pixel size (in wavelength) along the order, rebinning is the only possibility one has in order to merge adjacent orders. This effect is shown in Fig. 2 in which the pixel size (in nm) is shown as a function of wavelength along two adjacent orders of UVES.

1.1. Measuring lines

Once the spectrum has been "reduced" one has at his disposal a table of pairs (λ_i, F_i), where F_i may be actual measured flux, if the spectrum has been flux calibrated, or, more often, the number of counts. One next wants to "measure lines", i.e. for the spectral lines which can be detected in the spectrum, measure, at least, their wavelength position and their equivalent width (hereafter EW). Line position can be measured in many ways, e.g. simply measuring the position of the lowest pixel in the line, which is not recommendable unless one is happy with a very crude measure, or by measuring the center of gravity of the line, which is better. Also the equivalent width can be measured in many ways starting from direct numerical integration of the line profile (very accurate for data with extremely high S/N ratios) to the measurement of the central depth of the line, suitably calibrated (see e.g. Norris et al. 2000). However a quick look at the recent literature will show that the method of choice is usually fitting a known profile to the observed line. Very often the profile chosen is a gaussian, but it may be any known instrumental profile, or a synthetic profile. In the future this will be the dominant choice, also thanks to the availability of automatic or semi-automatic codes, which can measure hundreds of lines in a few minutes, like the code `fitline` described in (François et al. 2003) or DAOSPEC (Stetson & Pancino 2005).

The fitting of the profile has the immediate advantage that it provides the line EW and central wavelength at the same time. Moreover the fitting technique can perform well even at rather low S/N ratios where methods such as direct integration or center of gravity perform very poorly. From the point of view of data analysis, fitting a gaussian or other profile to derive the EW is not different to the line profile fitting described in the next section, so read on. Here I simply want to provide a few warnings. Line profile fitting assumes the shape of the line is known (e.g. gaussian). Make sure you *know* what the line profile is, it is useless to fit with a gaussian a line which has strong wings (e.g. Mg I b triplet lines in solar-like stars) or to fit a single gaussian to something you know is a blend of two lines (e.g. the Li I D doublet !) or to fit a gaussian when your spectrograph has a distinctly non-gaussian profile (check your arc lines !). In this way you will avoid to introduce systematic errors which may be very difficult to trace back *a posteriori*. If the precise shape of the line cannot be predicted it is preferable to use direct integration which requires no knowledge of the line shape.

2. Line profile fitting

Line profile fitting constitutes a more general tool of spectrum analysis, while the measurement of EWs generally applies only to isolated lines we may apply line profile fitting also to line blends. Moreover an EW describes the line with a single number while the line profile contains considerable more information, including line broadening, line asymmetry etc... The prerequisite is to be able to compute a synthetic spectrum for the spectral region of interest. In the following I will assume this is the case and will not address the uncertainties in the synthetic spectrum which are the topic of several other talks at this meeting.

Our computed profile depends on many parameters and our fitting procedure aims at determining the values of the parameter(s) for which the computed profile *best* reproduces the observed profile. One clearly needs a practically implementable definition of optimum. Up to the recent past it has been common practice to use visual inspection to chose the best fitting profile. This is not as bad as at sounds, two experienced spectroscopists will, in most cases, chose very similar profiles as "best fitting". However this practice should in general no longer be considered acceptable because it does not allow to estimate the errors in the fitted parameters and cannot possibly be applied to the large number of high quality data which is being delivered by modern telescopes.

Mathematically speaking, the problem is to define a suitable distance in the space constituted by all the possible synthetic profiles (which are obtained by varying the fitting parameters within the allowed ranges) and then find the point in this space (the fitting profile) which has minimum distance from the observed profile. From the practical point of view your observed profile is constituted by N pairs (λ_i, y_i) and your synthetic profiles by an infinity of N pairs (λ_i, Y_i) were Y is a function of all the fitting parameters. Manageable implementations of a distance that I have tried are $\chi^2 = \sum \frac{(y_i-Y_i)^2}{\sigma_i^2}$ and $D = \sum \frac{|y_i-Y_i|}{\sigma_i}$. The fitting consists in finding the parameters which minimize one of these quantities.

A large literature exists on χ^2, least squares and related topics (see e.g. Press et al. 1992 and Bevington & Robinson 2003 and references therein) and of course a number of important theorems which allow to estimate the goodness of fit and the errors in the fitted parameters. This could suggest that it is better to use χ^2 in order to take advantage of these theorems. Unfortunately all these theorems *do not apply to spectra*. This because the first hypothesis under which all the theorems are derived is that the data points must be *independent*. This is never the case for spectra, in most spectrographs the slit projects onto at least two pixels, which means that adjacent pixels (data points) are *correlated*. For undersampled spectrographs it is never the case that the slit projects *exactly* on one pixel, again this produces correlation in adjacent pixels. Even if we built deliberately a spectrograph in which the slit projects on one pixel the cross talk on the detector will end up correlating adjacent pixels. Moreover in general we rebin our spectra,

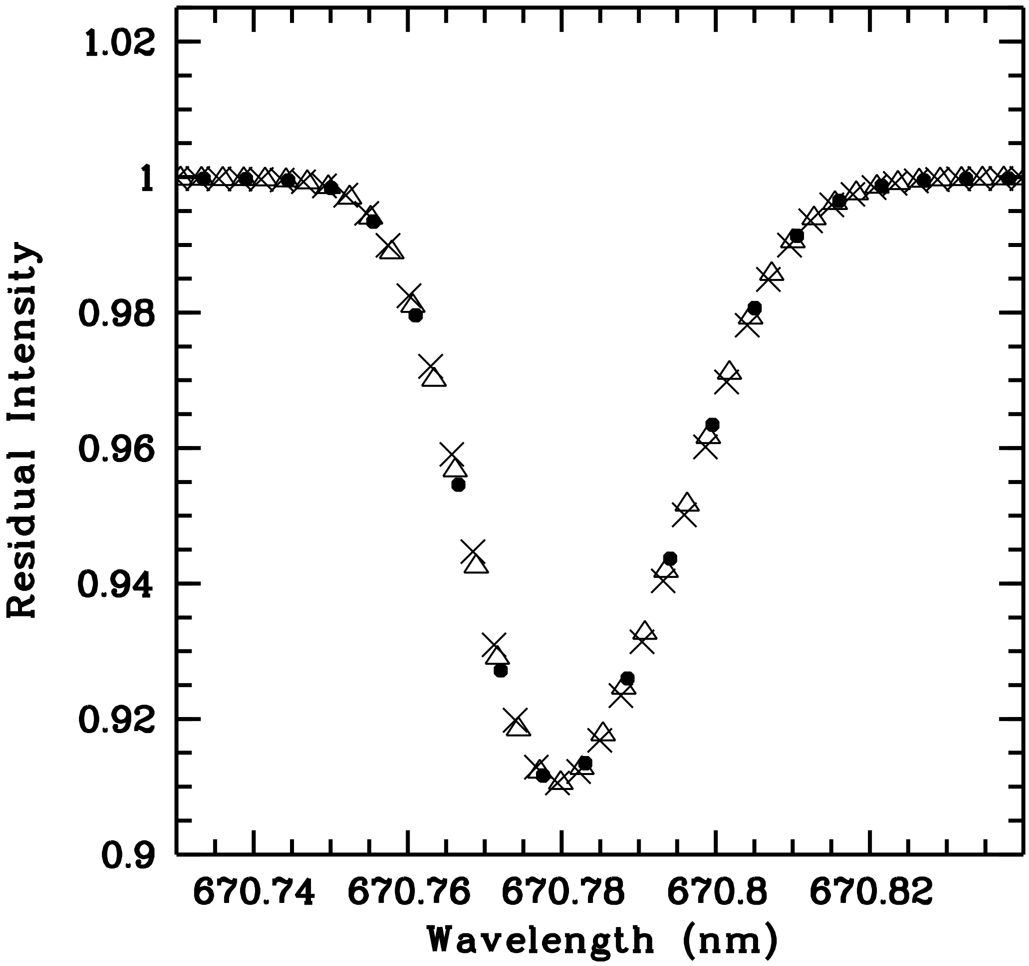

Fig. 4. The same synthetic profile sampled in different ways: triangles, the 573nm setting upper CCD; $\times$, the 850nm setting, lower CCD; dots, the 850nm setting but with a 2×2 on-chip binning, the resolution is the same as in the previous cases.

thus introducing a strong correlation among adjacent pixels. Therefore χ^2 may be conveniently used to estimate parameters, however χ^2 theorems to estimate errors do not apply.

One could argue that minimizing the absolute deviation D defined above is likely to be more robust than χ^2. In practical cases with real spectra when I tried to use both methods I found no appreciable difference in the fitted parameters nor in the execution times.

A few words on the fitting parameters. In principle these are all the atmospheric parameters ($T_{\rm eff}$, log g, ξ, chemical abundances) plus macroturbulence, rotation, radial velocity and, since we generally work on normalized spectra, the continuum level. In practice we use only the few which are of interest and keep the others fixed. For example I use the wings of Hα to determine $T_{\rm eff}$ for G dwarfs and then the only fitting parameter is $T_{\rm eff}$ the other being kept fixed. Very often I want to determine abundances and then the other atmospheric parameters are fixed, but macroturbulence, rotation and radial velocity should be fitted. In some cases one wants also to fit the isotopic

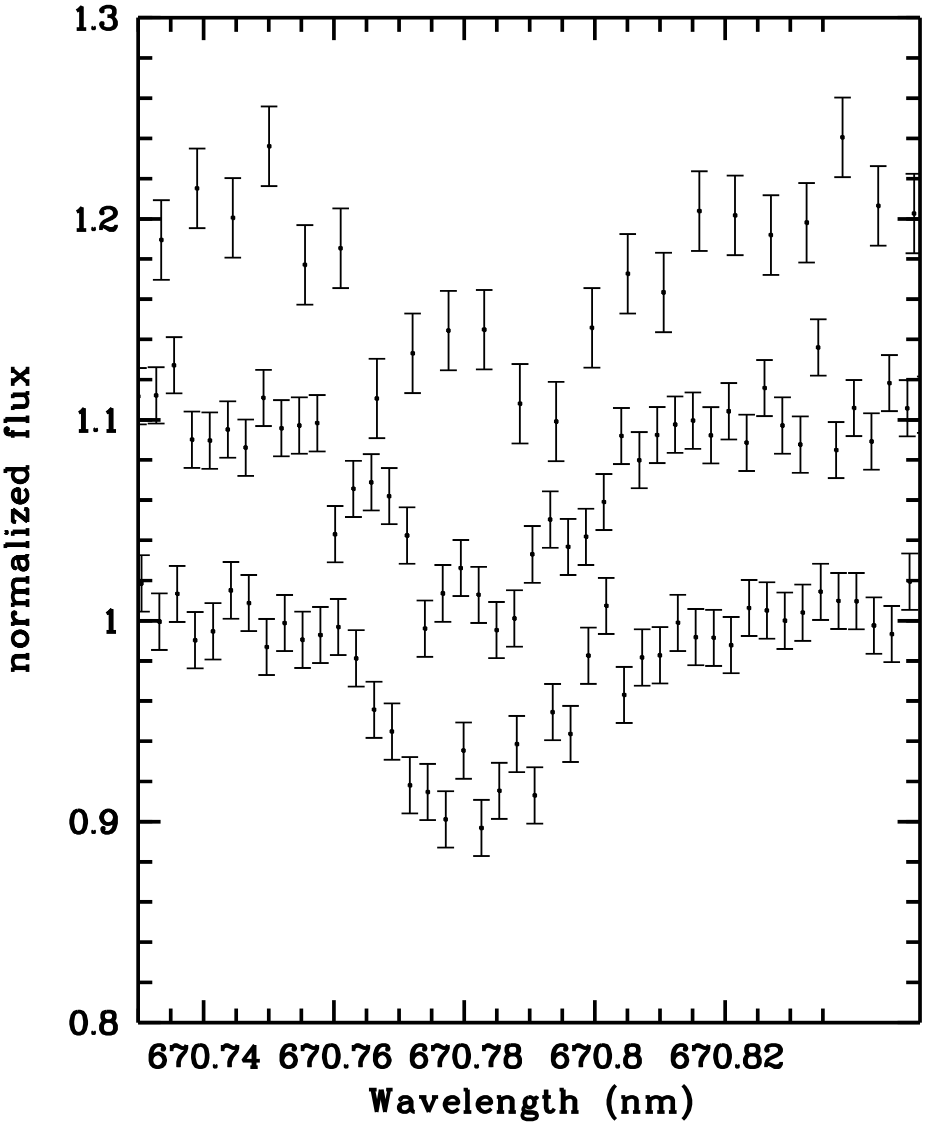

Fig. 5. Three realizations of the noise injection to the same synthetic profile, two profiles have been offset by 0.1 in normalized flux in order to avoid confusion: bottom profile, the 573nm setting upper CCD; middle profile the 850nm setting, lower CCD; upper profile the 850nm setting but with a 2×2 on-chip binning, the resolution is the same as in the previous cases.

ratios, see Cayrel et al. (1999) for a thorough discussion of this case. Generally one assumes the resolution of the spectrograph is known, and convolves the synthetic spectrum with the known instrumental profile before computing the χ^2. In practice one often finds the widths of the lines of slowly rotating stars (which should be dominated by instrumental broadening) to be larger than the width of the arc lines. This is often due to a slight defocusing of the spectrograph due to mechanical or thermal drifts occurred between the time when the arc was

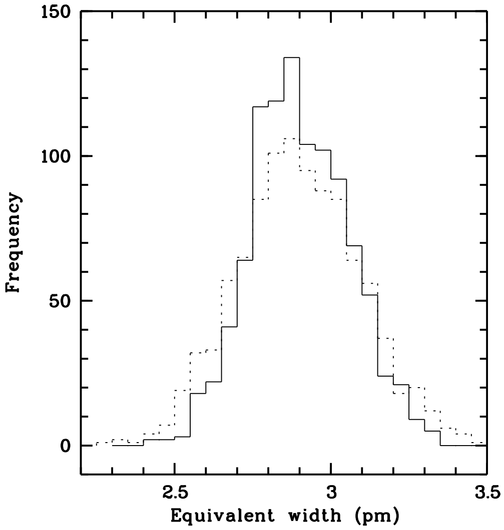

Fig. 6. Histogram of the fitted EWS by the "no rebinning", solid line, and the "rebinning", dotted line, procedures in the case in which the 2 spectra being combined have different physical sizes.

taken (usually in the afternoon before the observations or the morning after, with UVES) and the time of the observation. Occasionally it happens also that the lines are sharper than the arc lines, usually this happens when the seeing is considerably less than the slit width (e.g. 0.″5 seeing with a 1″ slit) and the resolution is fixed by the seeing rather than by the slit width. These situations are easily handled by simply including the instrumental broadening as a free parameter in the fitting procedure.

The minimum should always be sought numerically, there are many robust minimizers which can be taken off the shelf. I have a very positive experience with `MINUIT` (James 1998) which is freely available from CERN and is a multi-method minimizer, but also with the fail-safe downhill simplex method as implemented in `amoeba` (Press et al. 1992). My experience is it is not necessary to use very sophisticated methods. Pathological cases, with flat χ^2 minima, or local minima adjacent to absolute minima will in general cause trouble even to very sophisticated methods. On a present day laptop computer fitting a line profile with 5 to 10 free parameter should take a fraction of a second.

3. Rebinning the spectra

The question I want to address now is: does the rebinning introduce any limitation in the use we make of the data ? If so is there any way to avoid rebinning ? If the rebinning is done by properly oversampling the data it does not introduce any artifact. The practice of adding rebinned spectra may however have some undesirable effects: consider for example a case in which I add three spectra, one of which has several pixels spoiled by cosmic ray hits; if I add the three spectra all the wavelength range in which one of the three spectra was bad will be ruined, in spite of the fact that MOST of the spectra were good there. As stressed above the rebinning process introduces a correlation among pixels which prevents us from using the χ^2 theorems to estimate errors. If one is given a spectrum and does not know if the data has been rebinned or not one may compute the auto-correlation function, this must show a peak at 0, if the peak shows significant signal beyond 1 pixel, this means the pixels are correlated, the spectrum has been rebinned or smoothed with some kind of filter. An example of this procedure is shown in Fig. 3

We may apply the χ^2 fitting to the rebinned data however we cannot tell: 1) if the fit obtained is good or bad; 2) the error in the fitted parameters. These two features make the use of rebinned data highly undesirable. From a pragmatic point of view we may circumvent the problem by using a Monte Carlo technique. Assuming that we understand reasonably well the noise in the data we may take the "fitted data", inject noise and perform the fitting a large number of times ($\sim$ 1000 is typically sufficient). The σ in the distribution of any fitted parameter may be taken as the "error" in that parameter. Competing models may discriminated by choosing the one which has the smallest "error" in the parameters, although ambiguous cases are likely to arise.

In Fig.4 I show practically an example of how the Li I D doublet is sampled by UVES with three different instrument setups (573nm 1×1CCD binning, 850nm1×1CCD binning, 850nm2×2CCD binning), all of which provide the same spectral resolution. In Fig.5 I show the a realization of noise injection in the three profiles, the S/N ratio is 70 in all three cases.

3.1. No rebinning

Can we do something else ? Do we really need the rebinning ? Can we do without it ? If we examine carefully all of the above cases for rebinning we conclude that the only reason for the rebinning is to add together the signal contained in different physical pixels, which alas, refer to slightly different wavelengths. The only reason to do this is to increase the S/N ratio and hence, hopefully, make the errors on the fitted parameters smaller. However on closer examination the χ^2 technique does provide a way to combine the data, thus obtaining the desired improvement on the errors in the derived parameters, without rebinning the spectra.

Let us change slightly the notation: let us assume that we have N spectra of the same object, the data set may be described as $\{w_{ij}, y_{ij}\}, i = 1, M_j, j = 1, N$ where M_j is the number of pixels in the $j-th$ spectrum w_{ij} is the wavelength corresponding to the $i-th$ pixel of the $j-th$ spectrum and y_{ij} is the corresponding flux. This data-set may arise in any way: from different rows of a detector in presence of slit-curvature, from overlapping orders of echelle spectra, from spectra observed on different nights and even with different spectrographs, or any combination of the above. We assume that we may compute the value Y_{ij} of the model, for any desired w_{ij}, an assumption which is always satisfied in practical cases. Let us define

$$\chi^2 = \sum_j \sum_i \frac{(y_{ij} - Y_{ij})^2}{\sigma_{ij}^2}$$

this is indeed a χ^2 to which all theorems apply, in fact all data points are independent. This formula is in fact so general that it may even allow to combine spectra of different resolution, which with the usual "rebinning" approach is problematic, since it requires that before co-addition the spectrum of higher resolution be degraded to the lower resolution. This is possible but results in the loss of information.

4. A practical example

I want to show now a practical case and compare the results of the "rebinning" approach versus "no rebinning". Let us consider the region 670.73 nm to 670.85 nm, containing the Li I D resonance doublet. Assume we have two spectra one covered by the UVES setting centered at 573 nm (MIT CCD), the other covered by the UVES setting centered at 850 nm. The set of w_{ij} has been taken from two wavelength solutions found for real data. The MIT CCD spectrum, which we shall call UP, has 44 pixels in this region. The EEV CCD, which we shall call LOW has 43 pixels. We assume both spectra to have the same resolution of 7 km/s, the slit is therefore oversampled by the detector.

I computed a synthetic spectrum of the Li doublet, which has an EW of 2.90 pm, and used it to produce simulated "observed" spectra in several ways, by injecting Poisson noise, so that the resulting S/N =70. I compared the results of the "no rebinning" procedure to those of a procedure in which prior to fitting the "data" was rebinned to a constant step of 0.001 nm and, if necessary, combined. Each case was run for 1000 times and the results stored. The χ^2 minimization was performed using MINUIT. The results are summarized in Table 1, the mean EWs and the standard deviations of the Monte Carlo samples are given as in the second column, while formal errors from the χ^2 in the "rebinning" and "no rebinning" case are found in the third and fourth columns.

4.1. One spectrum UP

As expected in this case the "no rebinning" and the rebinning approach provide the same EW and the same dispersion. $< EW >_r =$ 2.909 ± 0.1658pm, while $< EW >_{nr} =$ 2.909 ± 0.1659pm. While the error estimated by the "no rebinning"procedure is in good agreement with the observed dispersion in EWs, the "rebinning" procedure underestimates the error by

Table 1. Results of Monte Carlo simulations. The σ are the formal errors from the χ^2

case	$< EW_r >$ pm	$< EW_{nr} >$ pm	$< \sigma_r >$ pm	$< \sigma_{nr} >$ pm
U	2.909 ± 0.1658	2.909 ± 0.1659	0.0826	0.1568
UL	2.901 ± 0.1181	2.901 ± 0.1183	0.0579	0.1107
UL2	2.899 ± 0.1942	2.902 ± 0.1547	0.0692	0.1402

roughly a factor of 2. $< \sigma >_{nr} >= 0.157$pm, while $< \sigma >_r >= 0.082$pm.

4.2. Two spectra: one UP and one LOW

In this case in the "rebinning" procedure the spectra are summed before submitting them to the fitting. As expected since the total amount of information is increased the mean value is closer to the true value and the dispersion is smaller $< EW >_r = 2.901 \pm 0.1181$pm and $< EW >_{nr} = 2.901 \pm 0.1183$pm. Also in this case the error estimated by the "no rebinning" procedure is close to the observed dispersion while the error estimated by the "rebinning" procedure is a factor of 2 smaller: $< \sigma_{nr} > = 0.111$pm, while $< \sigma_r > = 0.058 >$pm.

4.3. Two spectra: one UP and one LOW with 2×2 CCD binning

Here is a case in which the two procedure give remarkably different results. I assumed that the LOW spectrum was observed with a 2×2 on chip binning. This binning does not reduce the resolution, however it halves the number of pixels. $< EW >_r = 2.899 \pm 0.1942$pm and $< EW >_{nr} = 2.901 \pm 0.1547$pm. The pattern of the estimated errors is the same as in the above cases.

4.4. Discussion

The results of this exercise are in some respect comforting, in some other discomforting. It is good to find out that in simple cases the rebinning of data has no effect on the estimated EW. It is bad to discover that rebinned data is doing a very poor job for a complex case, in which the physical sizes of the pixels of the two spectra are different. The histogram in this case (Fig. 6) shows clearly that the distribution around the mean value is much wider than in the "no rebinning" case. What is even worse is that the dispersion is *larger* than what was obtained by fitting only *one* of the two spectra. So not only the "rebinning" procedure is unable to take advantage of the extra information contained in the second spectrum, but it actually results in larger errors, although, it must be stressed, the *mean value* of the EW is closer to the true value.

5. Conclusion

From the above discussion we may conclude that line-profile fitting should be used with due care. In particular I emphasize that the theoretical profile to be fitted should be chosen with a good *a priori* understanding of what the data to be fitted is (isolated line or blended, instrumental profile, rotational profile, etc...). Errors should be estimated using Monte Carlo techniques. Concerning the issue of rebinning the spectra I have shown that for the data analysis this is not in general necessary, therefore "no rebinning " should be preferred. Only in the case in which the spectra to be combined are very similar in binning and S/N ratio the "rebinning " does just as good and the error may be conveniently estimated by a Monte Carlo simulation. Possibly the superiority of the "no rebinning" approach breaks down in the very low S/N regime, but this has to be still investigated.

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